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Optimization of SO_2 Scrubber using CFD Modeling

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Abstract

The reduction of environmental contaminants that contribute to smog and soot is a worldwide goal that has seen an increased focus in recent years. In the United States, for example, it is estimated that by 2014 new rules will lead to a 71% reduction of sulfur dioxide emissions and 52% of nitrogen oxide emissions as compared to 2005 level. Thus, medium-sized plants (100-500MW) that currently do not have flue gas desulfurization (FGD) units or selective catalytic reduction systems (SCRs) will be required to adapt. Similar emission reduction efforts are expected to be adopted globally, albeit at different levels. Wet-scrubber FGD is characterized as one of the most effective SO_2 removal techniques with low operating costs. However, capital cost for implementation is considered high. Hence an effective optimization procedure is required to reduce these capital costs of conversion.
Power plants commonly use a lime slurry spray reaction to reduce SO_2 emissions. Control of the droplets throughout the tower geometry is essential to ensuring maximum reduction while minimizing scale. The liquid slurry is known to have density, surface tension and viscosity values that deviate from standard water spray characteristics, which complicates process optimization. In order to improve the scrubber, nozzle characteristics and placement must be optimized to reduce the cost of the system implementation and mitigate risks of inadequate pollution reduction. A series of large flow rate, hydraulic, hollow cone sprays were investigated for this study.
A Computational Fluid Dynamics (CFD) model was used to examine potential scrubber designs for optimization of the system. Nozzle parameters were modeled to allow particle tracking through the system. An ANSYS Fluent Lagrangian particle tracking method was used with heat and mass transfer. The alkaline sorbent material and SO_2 reaction is modeled to determine uniformity and efficacy of the system. Volumetric chemistry mechanisms were used to simulate the reaction. These results demonstrate the expected liquid-gas interaction relative to the system efficiency. Drop size, liquid rheology, and spray array layout were examined to achieve SO_2 removal above 90%. Wall impingement and flow pattern results were evaluated due to their impact in minimizing equipment plugging and corrosion required as for long-term scrubber utilization.

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Keywords: Flue Gas Desulfurization (FGD), Pollution control, Sprays;

1. Introduction

The reduction of environmental contaminants that contribute to smog and soot is a worldwide goal. As restrictions on emissions increase around the world, there is a global need for upgrades or additions to pollution control systems. Based on current regulation projections, medium-sized plants (100-500MW) that currently do not have flue gas desulfurization (FGD) units or selective catalytic reduction systems (SCRs) will be required to adapt in a short timeframe. Wet-scrubber FGD is characterized as one of the most effective SO_2 removal techniques with low operating costs. However capital cost for implementation is considered high. Hence an effective optimization procedure is required to reduce these capital costs of conversion.

Process improvement and optimization is a constantly ongoing effort. Power plants commonly use a lime slurry spray reaction

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to reduce SO_2 emissions. Droplet size introduced into the tower is essential to ensuring maximum reduction while minimizing scale. The liquid slurry is known to have density, surface tension and viscosity values that deviate from standard water spray characteristics, which complicates process optimization. The improvements made in nozzle design and liquid atomization, in recent years, have provided the possibility of process optimization like never before. In order to improve the scrubber, nozzle characteristics and placement must be optimized to reduce the cost of the system implementation and mitigate risks of inadequate pollution reduction. In situ analysis would provide the best assessment of a spray's characteristics in the tower, however often this is cost prohibitive or not physically possible. In lieu of inline optimization, computational fluid dynamics (CFD) projects for this type of application have become very useful. With CFD, gas conditioning process engineers are able to assess the spray quality within the actual spray process region.

Spraying Systems Co. has the unique combination of testing and modeling expertise that allowed for a rigorous validation of spray modeling techniques often used to simulate un-testable situations. This body of work relates to the analysis of various injectors to examine their efficacy in SO_2 reduction, using a lime slurry injection. The nozzles were characterized using Phase Doppler Interferometry (PDI) to determine drop size distribution and velocity at various operating conditions. This data is used to provide accurate input to model the FGD process.

Nomenclature

u_θ	velocity in the direction of (m/s)
A	radius of (m)
B	position of
C	further nomenclature continues down the page inside the text box
D_0	bulk diffusion coefficient (m/s)
C_g	mean reacting gas species concentration in the bulk (kg/m3)
C_s	mean reacting gas species concentration at the particle surface (kg/m3)
R_c	chemical reaction rate coefficient (units vary)
A_p	particle surface area (m²)
Y_j	mass fraction of surface species *j* in the particle
η_r	effectiveness factor (dimensionless)
$\mathcal{R}_{j,r}$	rate of particle surface species reaction per unit area (kg/m².s)
$\bar{\mathcal{R}}_{j,r}$	Rate of particle surface species depletion (kg/s)
p_n	bulk partial pressure of the gas phase species (Pa)
$D_{0,r}$	Diffusion rate coefficient for reaction *r*
$\mathcal{R}_{\mathrm{kin},\,r}$	kinetic rate of reaction r (units vary)
N_r	apparent order of reaction r
Greek symbols	
γ	stoichiometric coefficient
δ	Boundary layer thicknesses (m)
Subscripts	
r	radial coordinate

2. Equipment and Methods

2.1. Test Setup and Data Acquisition

For drop sizing, the nozzle was mounted on a fixed platform in a vertical downward orientation. The data was acquired at 600mm downstream of the nozzle exit orifice. Drop size and velocity information was collected at various operating conditions. Multiple points throughout the spray plume were measured with a mass and area weighted average reported for comparison purposes.

A two-dimensional Artium Technologies PDI-200MD [9, 10] system was used to acquire drop size and velocity measurements. The solid state laser systems (green 532 nm and red 660 nm) used in the PDI-200MD are Class 3B lasers and provide 50-60mWatts of power per beam. The lasers were operated at an adequate power setting to overcome interference due to spray density.

The transmitter and receiver were mounted on a rail assembly with rotary plates; a 40° forward scatter collection angle was used. For this particular test, the choice of lenses was 1000mm for the transmitter and 1000mm for the receiver unit. This resulted in an ideal size range of about 4.0µm – 1638µm diameter drops. The optical setup was used to ensure acquisition of the full range of drop sizes, while maintaining good measurement resolution. The particular range used for these tests was determined by a preliminary test-run where the DV0.5 and the overall droplet distribution were examined. For each test point, a total of 10,000 samples were acquired. The experimental setup can be seen in Figures 1 and 2.

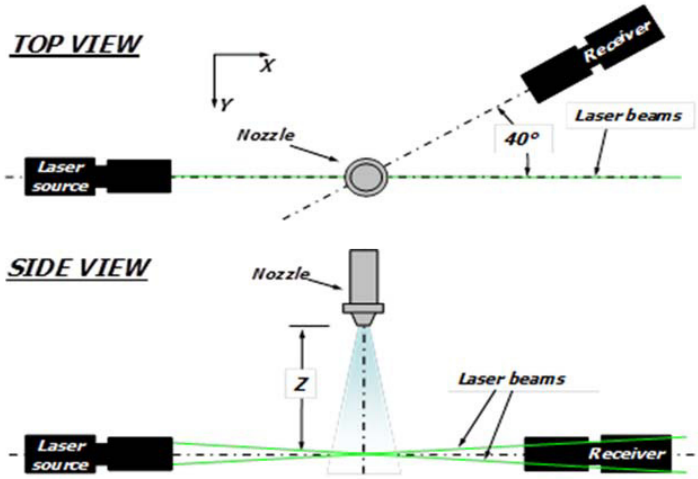

Fig 1. Illustration of PDI layout for drop size and velocity data acquisition.

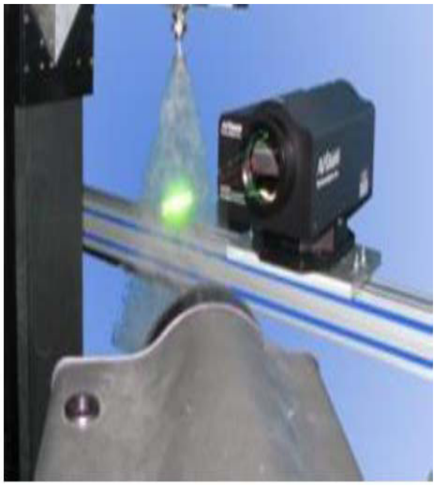

Fig 2. Illustration of PDI during experiment

The $D_{V0.1}$, $D_{V0.5}$, D_{32}, and $D_{V0.9}$ diameters were used to evaluate the drop size data. This drop size terminology is as follows:

$D_{V0.1}$: is a value where 10% of the total volume (or mass) of liquid sprayed is made up of drops with diameters smaller or equal to this value.

D_{32}: Sauter Mean Diameter (also known as SMD) is a means of expressing the fineness of a spray in terms of the surface area produced by the spray. SMD is the diameter of a drop having the same volume to surface area ratio as the total volume of all the drops to the total surface area of all the drops.

$D_{V0.5}$: Volume Median Diameter (also known as VMD or MVD). A means of expressing drop size in terms of the volume of liquid sprayed. The VMD is a value where 50% of the total volume (or mass) of liquid sprayed is made up of drops with diameters equal to or smaller than the median value. This diameter is used to compare the change in average drop size between test conditions.

$D_{V0.9}$: is a value where 90% of the total volume (or mass) of liquid sprayed is made up of drops with diameters smaller or equal to this value.

By analyzing drop size based on these standardized drop statistics it is possible to objectively characterize the quality and effectiveness of this atomizing nozzle for the prescribed application.

2.2. Test Fluids and Monitoring Equipment

All testing was conducted using water and solution to simulate the fluid properties of lime slurry. Flow to the system was supplied using a high volume pump. The liquid flow rate to the injector was monitored with a MicroMotion flow meter and controlled with a bleed-off valve. The MicroMotion flow meter is a Coriolis Mass flow meter which measures the density of the fluid to determine the volume flow. The meter is accurate to 0.4% of reading. Liquid pressures were monitored upstream of the injector with a 0-1.03MPa, class 3A pressure gauge.

2.3. Injectors

Two types of injectors were evaluated to determine the effectiveness for this application. The injectors were full cone, narrow style injectors, of the Spraying Systems Co. FullJet style. The injectors were selected based on a target flow rate of 37.85 lpm flow. Multiple capacity sizes and configurations were used to achieve this design requirement.

3. Numerical Simulations

3.1. CFD Background

Computational Fluid Dynamics (CFD) is a numerical method used to numerically solve fluid flow problems. Today's CFD performs use extremely large number of calculations to simulate the behavior of fluids in complex environments and geometries. Within the computational region, CFD solves the Navier-Stokes equations (Figure 3) to obtain velocity, pressure, temperature and other quantities that may be required by a tackled problem. Recently CFD became a popular design and optimization tool with the help of commercially available software and advancing computer technology. The commercially available CFD package ANSYS FLUENT (version 14) was used for the simulation

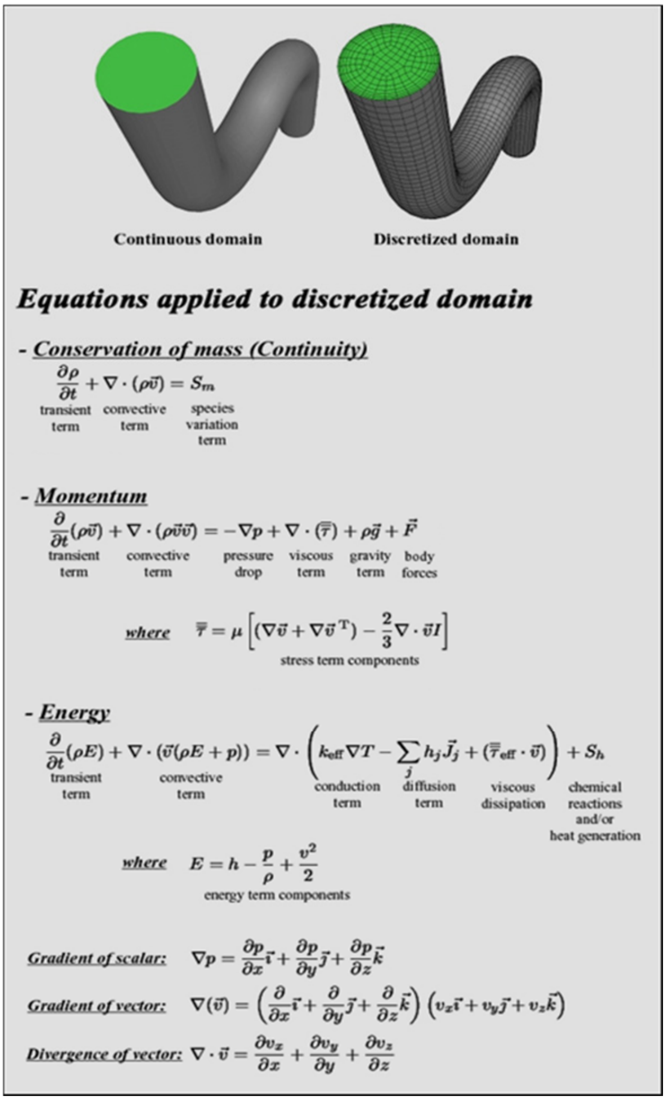

Fig. 3. CFD Governing Equations

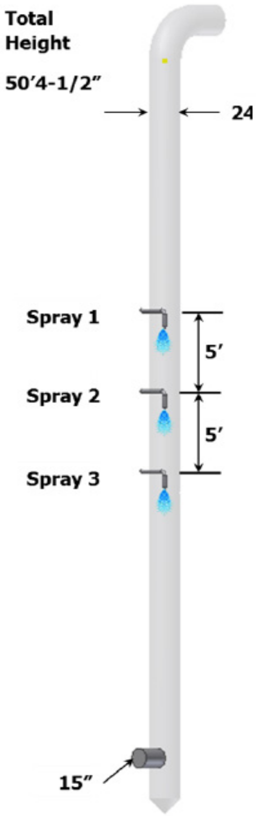

Fig. 4 CFD Scrubber Geometry

3.2. Simulation Description

Figure 4, shows a pilot wet absorber that has a capacity of 6 million Btu/hr. This geometry was used for the model of the high velocity absorber [1]. The absorber has a gas flow capability of 4000 acfm, with SO_2 concentrations up to 6000 ppmdv. The gas flow comes in from the inlet and continues through the absorber turn to the outlet. Liquid slurry enters from the injector(s) and moves out from the system at quenching zone. The importance of the pollutant removal process is determined through the observation of the gas liquid interactions at the tray, improved by optimization of the injector system.

Air and reacting gases inside the horizontal scrubber were set as primary phase flow (Eulerian approach). The primary phase used coupled models (momentum, turbulence, energy, species mixing and reaction) which required boundary conditions (BC's). This simulation consisted of inlet BC and outlet BC, set as "mass flow rate inlet" and "constant pressure outlet" respectively.

The calcium carbonate injection was set as secondary phase (Lagrangian approach) where its inlet BC are based on spray injection parameters as determined empirically. The Lagrangian particles were set using "wet combustion" models. The Lagrangian particles were tracked using Discrete Phase Model (DPM). During computation, heat and mass transfer was coupled between primary and secondary phases. CFD Multiple Surface Reaction Model set-up reaction kinetic parameters and factors are extracted and calculated through experimental results from Wang [6]and probabilities method from Krebs [7].

To generate the computation domain (mesh) for the scrubber shown in Figure 4, ANSYS workbench mesher (version 14) was utilized. The mesh consisted of (single injector configuration) 44003 polyhedral cells and 217150 faces; (two injector configuration) 53897 polyhedral cells and 273068 faces; (three injector configuration) 64391 polyhedral cells and 332411 faces, minimum cell size is 1e-5m. Due to its size and modeling complexity, the simulation required significant computer power and processing time. The walls had a common (standard) setup, with no slip, adiabatic (insulated) and reflect for the combusting particles.

3.3. Wet Combustion Particle Surface Reaction

Computational fluid dynamic (CFD) simulation is mainly using ANSYS Fluent Wet combustion particle surface reaction chemistry models, which have been developed and parametric tested during simulations. ANSYS Fluent can model the mixing and transport of chemical species by solving conservation equation describing convection, diffusion, and reaction sources by its multiple surface reaction models [4].

Reaction occurred in the bulk phase is dealt with volumetric reaction, and particle surface reaction. For gas-phase reactions, the reaction rate is defined on a volumetric basis and the rate of creation and destruction of chemical species. Particle surface reaction is used to model surface combustion on a discrete-phase particle. In the discrete phase model, modeling multiple particle surface reactions makes the surface species as a “particle surface species”.

The initial relationship for calculating particle-burning rates were presented and discussed by Smith [5]. The particle reaction rate, $\mathcal{R}$ (kg/m2·s), can be expressed as

$$\mathcal{R} = D_0 (C_g - C_s) = R_c (C_s)^N \qquad (1)$$

In above equation, the concentration at the particle surface, C_s, is unknown and eliminated as follows:

$$\mathcal{R} = R_c [C_g - \mathcal{R}/D_0]^N \qquad (2)$$

This equation has to be solved by an iterative procedure in Fluent, with the exception of the cases when N=1 or N=0, which can be written as

$$\mathcal{R} = \frac{C_g R_c D_0}{D_0 + R_c} \qquad (3)$$

In the case of N=0, if there is a finite concentration of reactant at the particle surface, the solid depletion rate is equal to the chemical reaction rate. If there is no reactant at the surface, the solid depletion rate changes abruptly to the diffusion-controlled rate. ANSYS Fluent will always use the chemical reaction rate for stability reasons.

Based on the above explanation, ANSYS Fluent uses the following equation to describe the rate of reaction r of a particle surface species j with the gas phase species n. The rate is given as

$$\overline{\mathcal{R}}_{j,r} = A_p \eta_r Y_j \mathcal{R}_{j,r} \qquad (4)$$

$$\mathcal{R}_{j,r} = \mathcal{R}_{kin,r}\left(p_n - \frac{\mathcal{R}_{j,r}}{D_{0,r}}\right)^N \qquad (5)$$

The effectiveness factor is related to the surface area, which can be used in each reaction in the case of multiple reactions.
$D_{0,r}$ is given as (6)

$$D_{0,r} = C_{1,r}\frac{\left[\left(T_p + T_\infty\right)/2\right]^{0.75}}{d_p}$$

The kinetic rate of reaction r is defined as (7)

$$\mathcal{R}_{kin,r} = A_r T_p^{\beta_r} e^{-\left(E_r/RT_p\right)}$$

The rate of the particle surface species depletion for reaction order $N_r = 1$ is given by

$$\bar{\mathcal{R}}_{j,r} = A_p \eta_r Y_j p_n \frac{\mathcal{R}_{kin,r} D_{0,r}}{D_{0,r} + \mathcal{R}_{kin,r}} \quad (8)$$

For reaction order $N_r = 0$,

$$\bar{\mathcal{R}}_{j,r} = A_p \eta_r Y_j \mathcal{R}_{kin,r} \quad (9)$$

The surface reaction consumes the oxidant species in the gas phase, also consumes or produces energy, in an amount determined by the heat of reaction. The particle heat balance during surface reaction is

$$m_p c_p \frac{dT_p}{dt} = hA_p\left(T_\infty - T_p\right) - f_h \frac{dm_p}{dt} H_{reac} + A_p \varepsilon_p \sigma\left(\theta_R^4 - T_p^4\right) \quad (10)$$

It includes the diffusion and convection control of the vaporization model.

4. Results (Experimental and Numerical)

4.1. Experimental Results

The results of the PDI measurements provide a representative characterization of the atomizer effectiveness at the 600mm downstream investigation location. As outlined and described in the above sections, the results from testing are provided in Table 1. The Volumetric Mean Diameter ($D_{V0.5}$) as well as other representative diameter statistics based on the volume flow is presented. These results allow the evaluation, qualitatively, of the dependence of drop size on the liquid flow rate and pressure.

Table 1. Drop Size and Velocity Results of Empirical Investigation

Nozzle ID	Units	1HH-SS 3070	1/2GG-SS 3030	1/2GG-SS 3030	1/2GG-SS 3030
Pressure (dP)	psi	82	111	40	71
DV0.5	micron	539	443	635	530
Distribution Parameter		2.5	2.5	2.5	2.5
Injected Flow	lpm	37.9	18.9	11.4	15.1
No. of Spray Levels		1	2	3	3

There are notable trends that persist throughout the data. With an increase in liquid feed pressure, there is a decrease in median drop size and an increase in mean drop velocity.

4.2. CFD Results

One to three injectors were evaluated in series to determine optimal design parameters. All simulations were performed with a consistent total mass flow rate of 37.9 lpm. The effect of the injector is evaluated to allow for a design with minimal waste and wall contact, to improve efficacy and decrease the required maintenance of the system. The results indicated the SO_2 mass fraction in each case and SO_2 removal for each case. Velocity magnitude and vertical velocity profile, discrete phase concentration and particle tracking is shown to better understand the flow behavior and pattern in the scrubber.

All cases achieve full SO_2 reduction as designed. Three-nozzle scrubber has the best SO_2 removal capability, based on calcium carbonate consumption. Similarly, the two-nozzle scrubber shows a greater removal than one-nozzle scrubber with less calcium carbonate consumption at the same supply quantity. This result indicates a trend relating smaller drop sizes to greater efficacy of SO_2 removal. Due to the relationship of drop size volume to surface area, with equivalent volume introduced into the system, it is possible to significantly increase surface area and associated surface reaction rate in the tower. Moreover, increasing spray zone flow distribution will lead to higher efficiency. The velocity behaviour exhibits less oscillation and recirculation than the in the three-nozzle scrubber at the same high inlet velocity. However, it causes adverse results with respect to wall wetting. It should be noted that there is an especially high concentration area formed around spray zone, which is greater than expected. Wall impingement may cause equipment erosion when injection fluid has corrosive property.

Table 2. SO_2 Scrubber CFD Simulation Species Data

Case Name	net species mass flow	O_2	SO_2	CO_2	$CaCO_3$ Slurry Consumption
1 Nozzle Injection	kg/s	0.01854	0.06198	-0.05213	26.97%
2 Nozzle Injection	kg/s	0.01592	0.06203	-0.04799	19.33%
3 Nozzle Injection	kg/s	0.01643	0.06187	-0.05345	18.89%

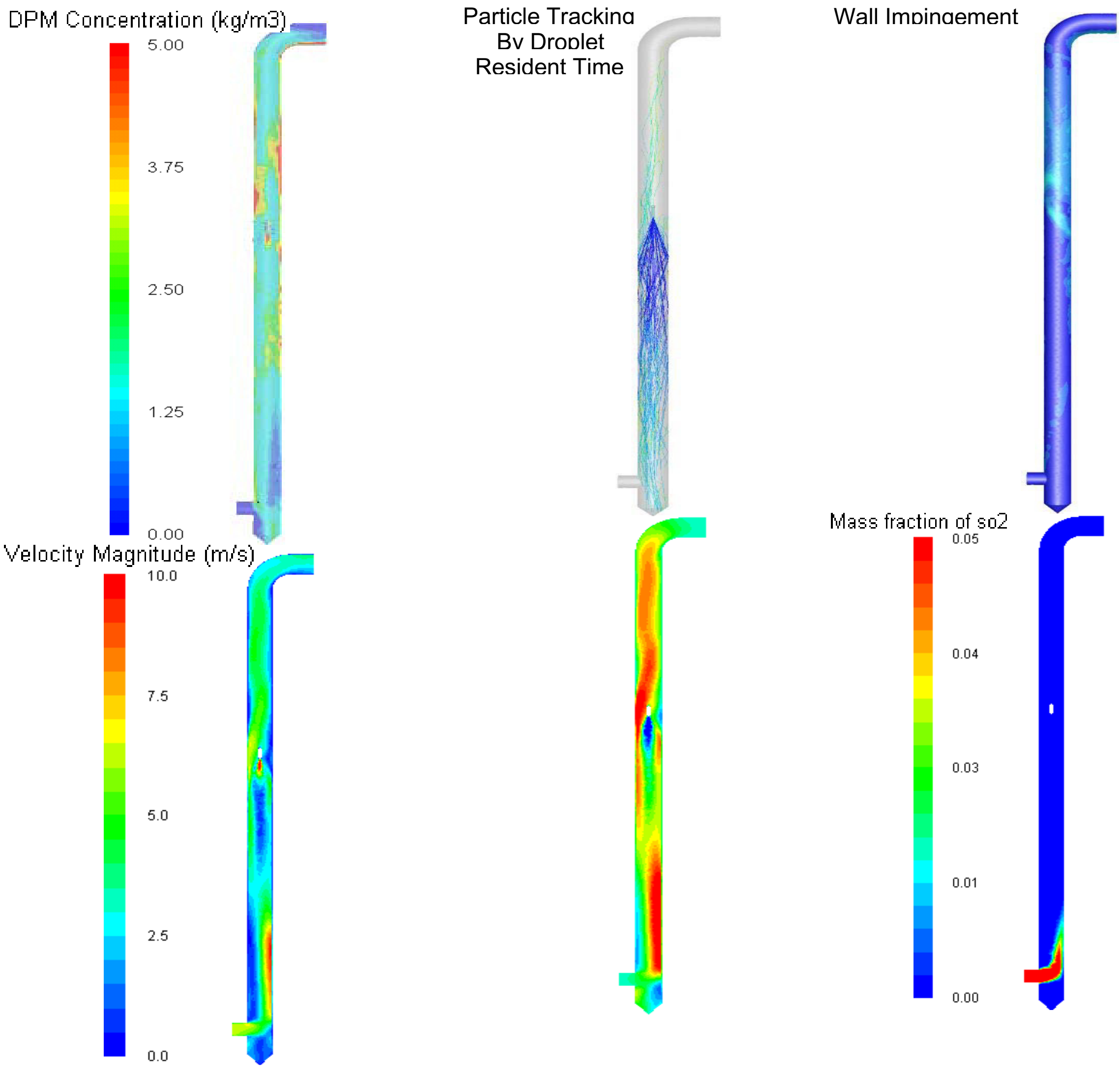

Fig. 5 Nozzle Injection Scrubber CFD Simulation Result

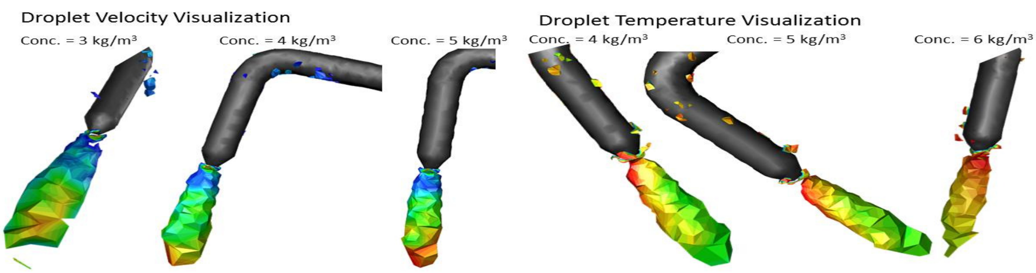

Fig. 6 Nozzle Injection Spray Visualization

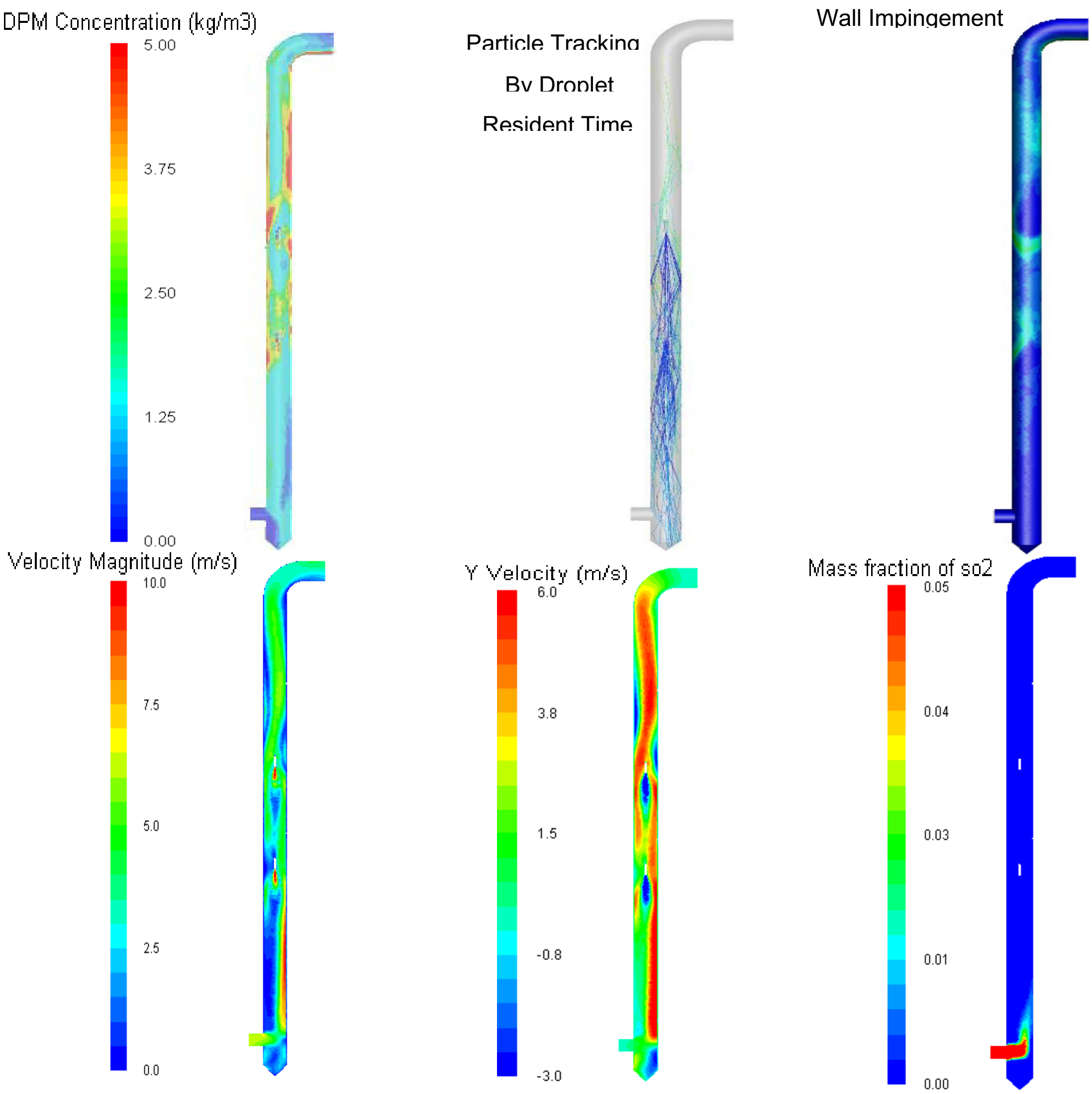

Fig. 7 Nozzle Injection Scrubber CFD Simulation

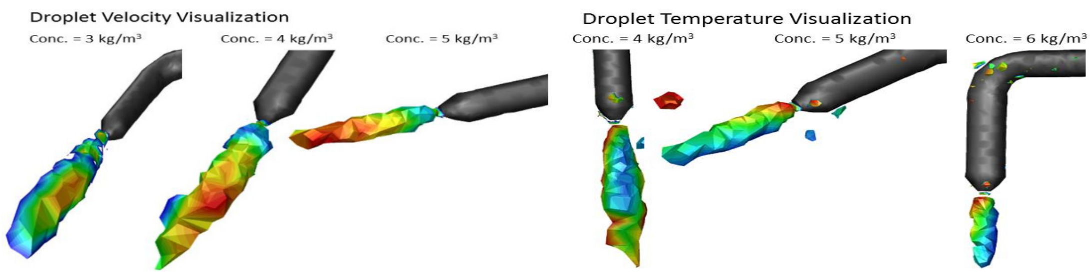

Fig. 8 Nozzle Injection Spray Visualization

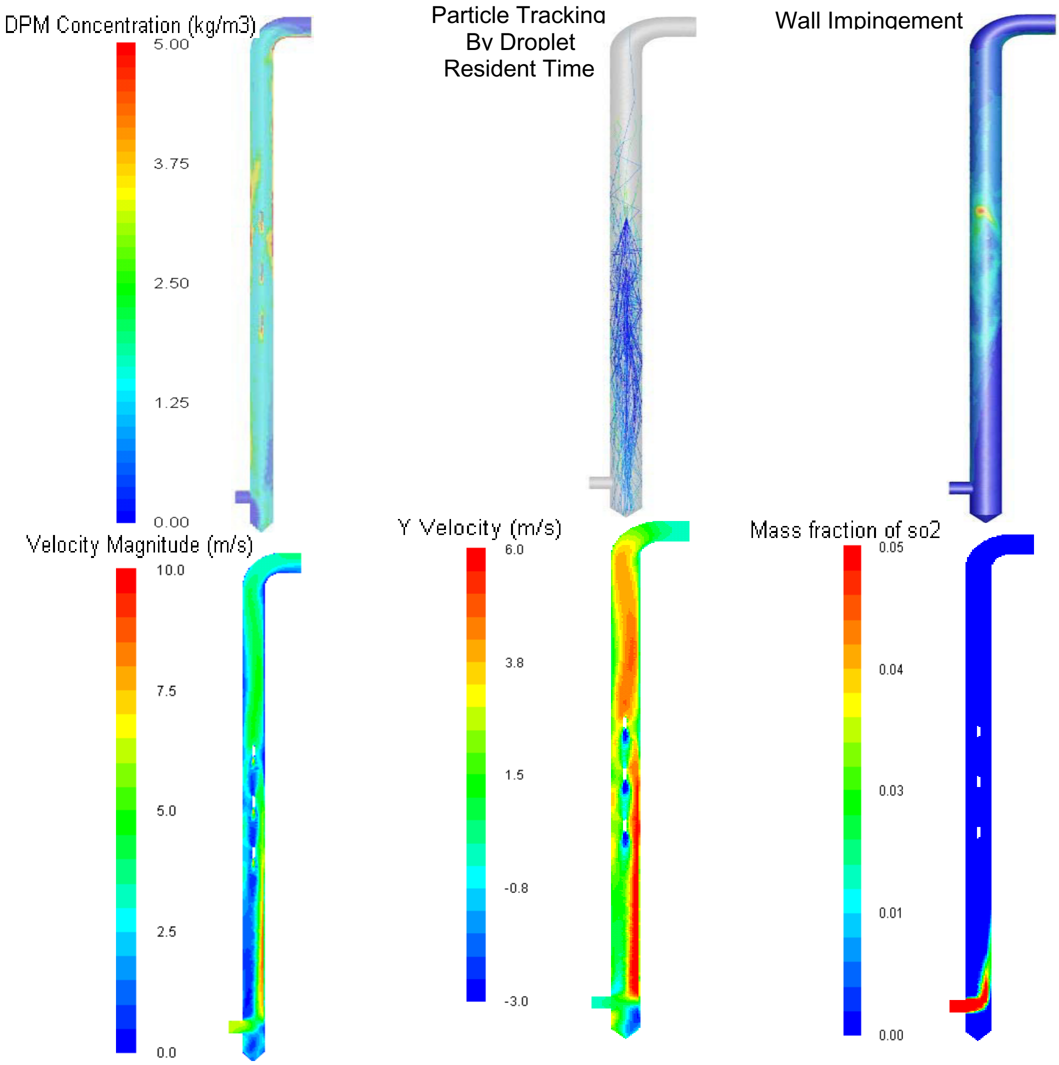

Fig. 9 Nozzle Injection Scrubber CFD Simulation Result

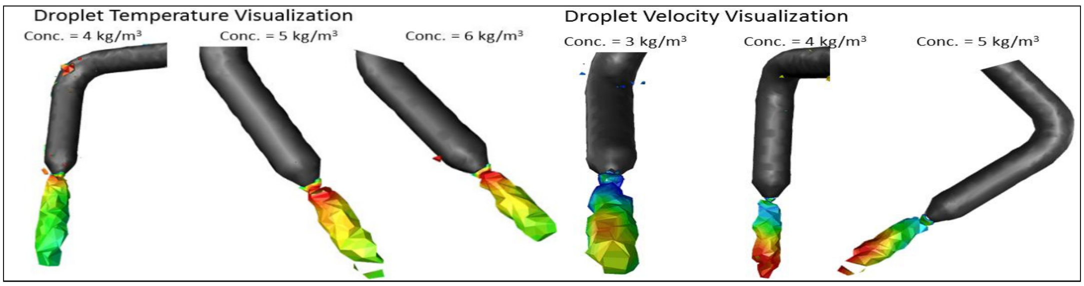

Fig.10 Nozzle Injection Spray Visualisation

In the three nozzle case, at 11.4 and 15.1 lpm supply quantity, more supply does not show better SO_2 reduction with smaller drop size. This may be due to the fact that the 11.4 lpm supply case has already achieved 18.89% of slurry consumption. The marginal reduction in drop size my not have significant effect on slurry consumption at this level. Also, the 15.1 lpm supply case has a total injection quantity of 45.4 lpm, when accounting for all injectors. This flow could be too much for the scrubber at this input condition, which might lead to less efficiency by slurry accumulation. These results may need further research to determine cause and effect of this result.

5. Conclusion

The results presented herein, represent a preliminary work for SO_2 removal based on different nozzle designs. From the net species mass flow table, it clearly shows the slurry consumption is below 50% for all the cases to remove targeted pollutants. The slurry injection quantity, effective usage research will be one of the further major subjects to improve scrubber efficiency.

Considering the slurry flow behaviour from the simulation result, high velocity inlet helped with the SO_2 fully removal, while it also caused concerns relating to undesirable wall interactions. Therefore, a range of different velocity inlet tests on the influence of nozzle selections, wall wetting and pollutant removal efficiency could make further improvements on this research.

Furthermore, as discovering the nozzle efficiency, several tests could be made to get relationship between nozzle supply quantity and nozzle provided droplet size for higher removal capability achievement. Through the optimal result, more nozzle designs can be made based on nozzle properties to develop spray behaviour and decrease erosion on the walls with the requirement of standard removal or even better. Future studies are planned to further develop computational models and increase understanding of FGD scrubber systems.

Acknowledgements

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Reference:

[1] P. J. Williams. "Wet Flue Gas Desulfurization Pilot Plant Testing of High Velocity Absorber Modules". Presented to EPRI-DOE-EPA Combined Utility Air Pollutant Control Symposium, 1999.
[2] Industrial Spray Products Catalog. Spraying System Co., B18-B31, 2010.
[3] Physical Data of Calcium Carbonate-water Suspensions. TAPPI TIP Category: Data and Calculations. TIP 0106-01, 2002.
[4] The Multiple Surface Reactions Model in Discrete Phase. ANSYS FLUENT Theory Guide for Version 14.0, 427-428, 2011.
[5] I.W. Smith. "The *Combustion Rates of Coal Chars: A Review*". *In 19th Symp. (Int'l.) on Combustion*. The Combustion Institute, 1045–1065, 1982.
[6] H. Wang, H. Xu, C. Zheng and J. Qiu. "Temperature Dependence on Reaction of CaCO3 and SO2 in O2/CO2 coal combustion". Journal of Central South University, Vol. 16, pp. 0845-0850, 2009.
[7] T. Krebs and G. M. Nathanson. "Reactive Collision of Sulfur Dioxide with Molten Carbonates". PNAS Early Edition, 2009.
[8] Lefebvre, A.W., Atomization and Sprays, Hemisphere Publishing Corporation,1989, p.1-78.
[9] Bachalo, W.D., "Experimental Methods in Multiphase Flows", International Journal on Multiphase Flow, Vol.20,Suppl. pp.261-295, 1994
[10] Bachalo, W.D., "A Method for Measuring the Size and Velocity of Spheres", by Dual Beam Light Scatter Interferometry, Applied Optics, Vol. 19, No.3, February 1, 1980.